Origins of Strength from Dislocation Dynamics

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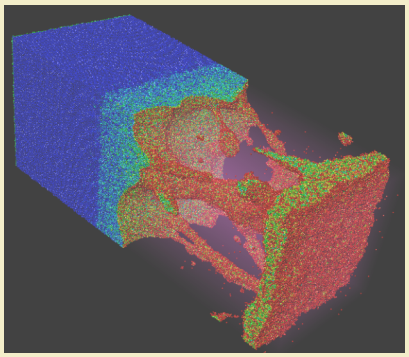
Experiments: **L. Hsiung, J. Florando, M. Leblanc**

Visualization: **R. Cook**

Dynamic of Metals project at LLNL

Funded by NNSA ASC Program

An accurate experimentally validated predictive model for metal strength under extreme conditions of pressure, temperature and strain rates

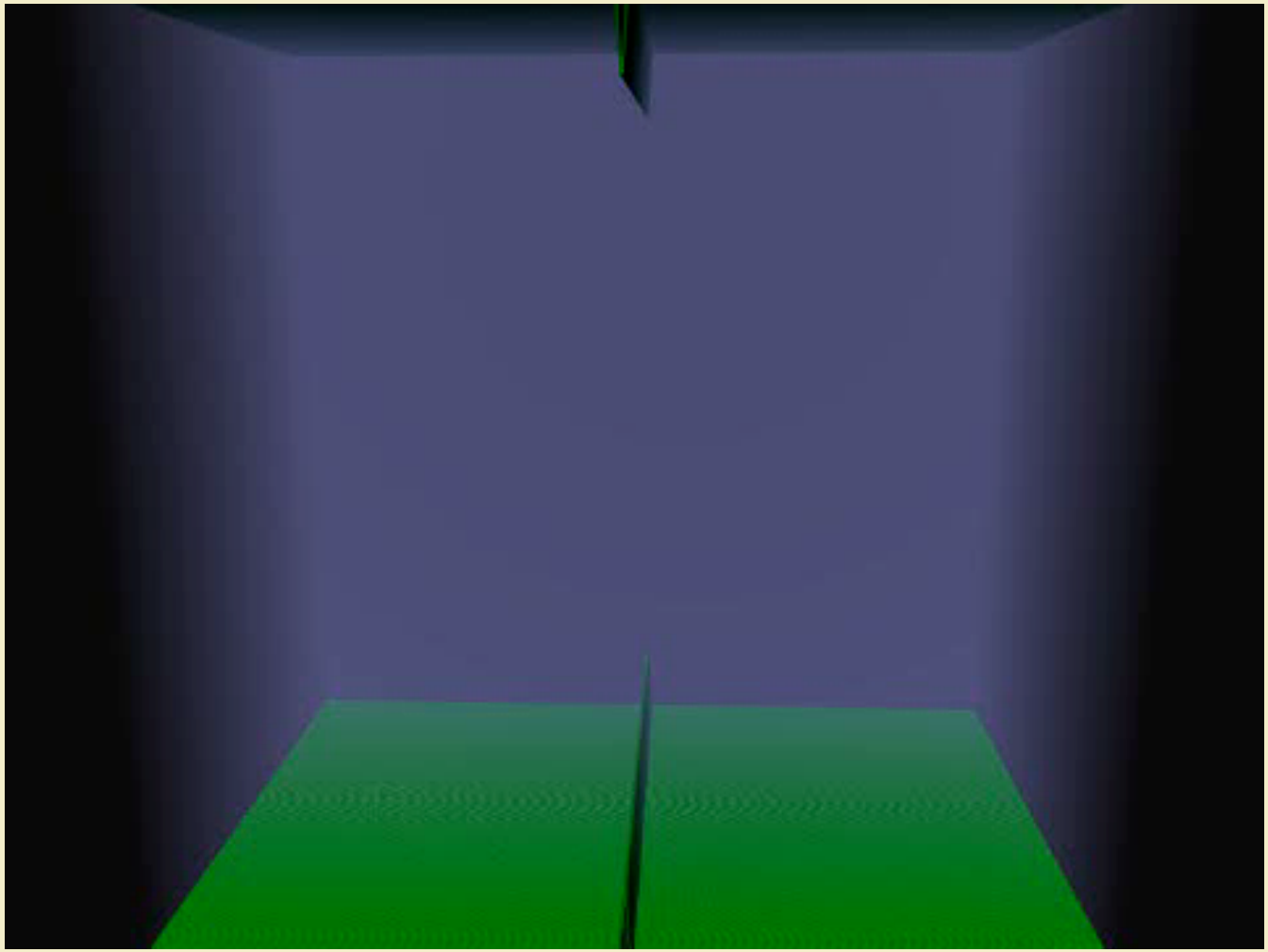


The premise: **compute strength directly as a result of the underlying atomistic mechanisms of material response**

The means: **multiscale simulations of material response**

A Molecular Dynamics simulation on ASC White

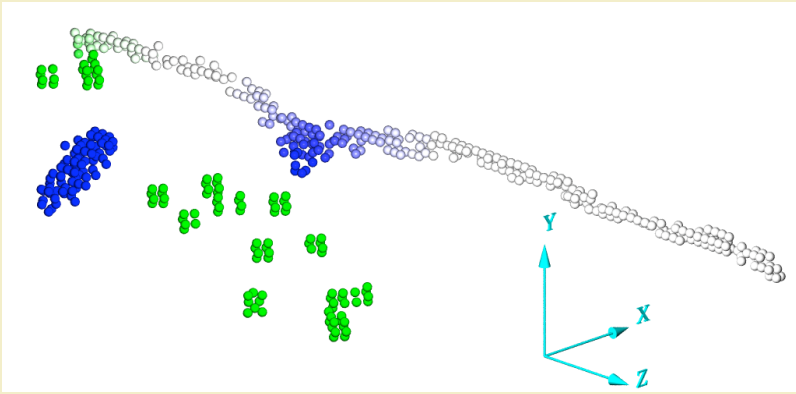
F. Abraham, M. Duchaineau *et al.* (2001)

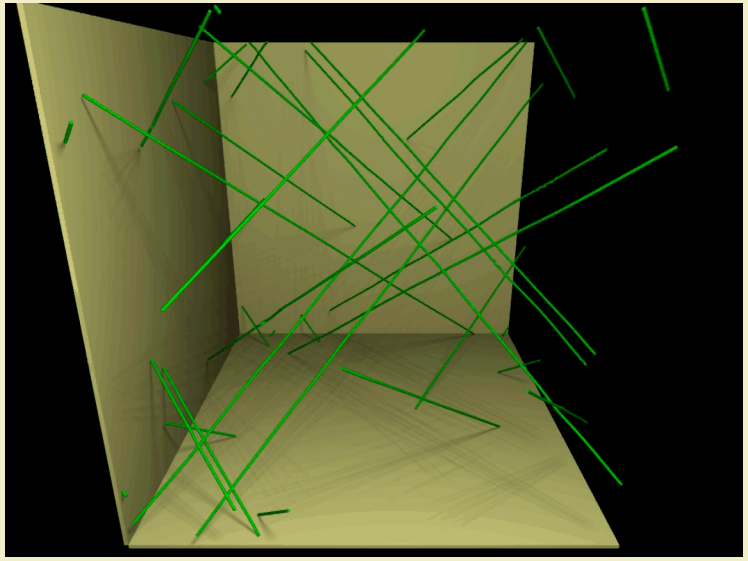


Coarse-grained approach of Dislocation Dynamics

"Crystals are like people, it's their defects that makes them interesting"

Understand and quantify how each line defect (a dislocation) responds to stress, temperature and pressure

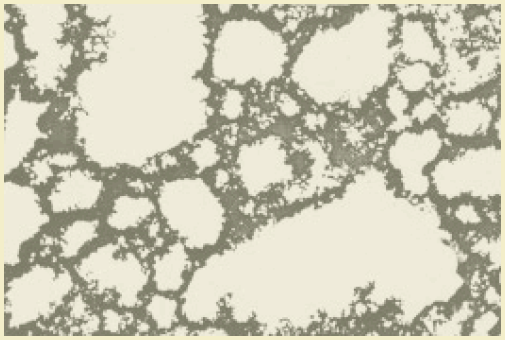




Assemble a simulation of many interacting lines to understand how collective motion of dislocations defines material strength

ParaDiS project (2001 – present)

Para-llel ***Di***-slocation ***S***-imulator



DD challenges

extreme computational cost - tens of millions of flops/DOF

handling of the evolving topology of dislocation networks

extreme spatial and temporal heterogeneity – load balancing

etc

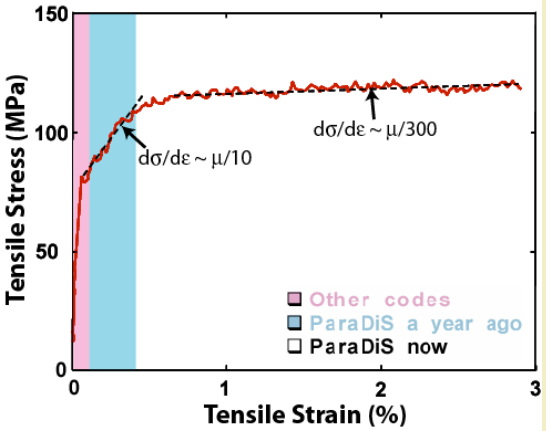
***ParaDiS* code:**

fully parallel, efficient dynamic load balancing

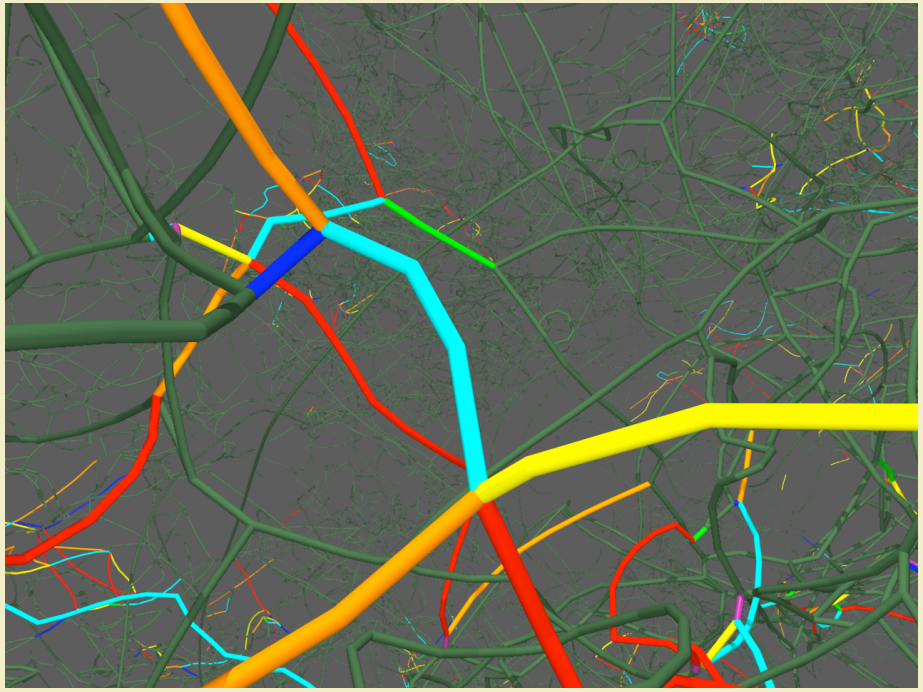
good scaling on massively parallel computers (Thunder, BG/L)

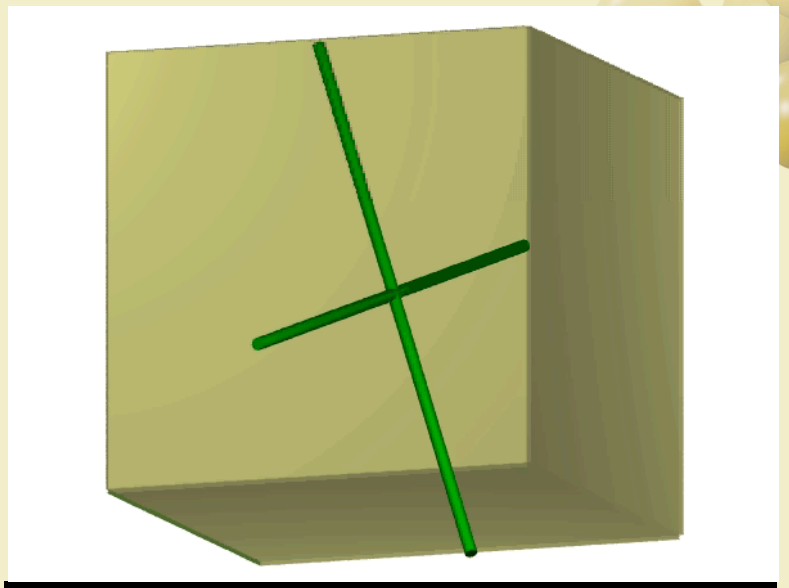
orders of magnitude larger and longer simulations

first ever meaningful simulations of crystal strength



Multiple slip causes many-body dislocation reactions
Multi-junctions

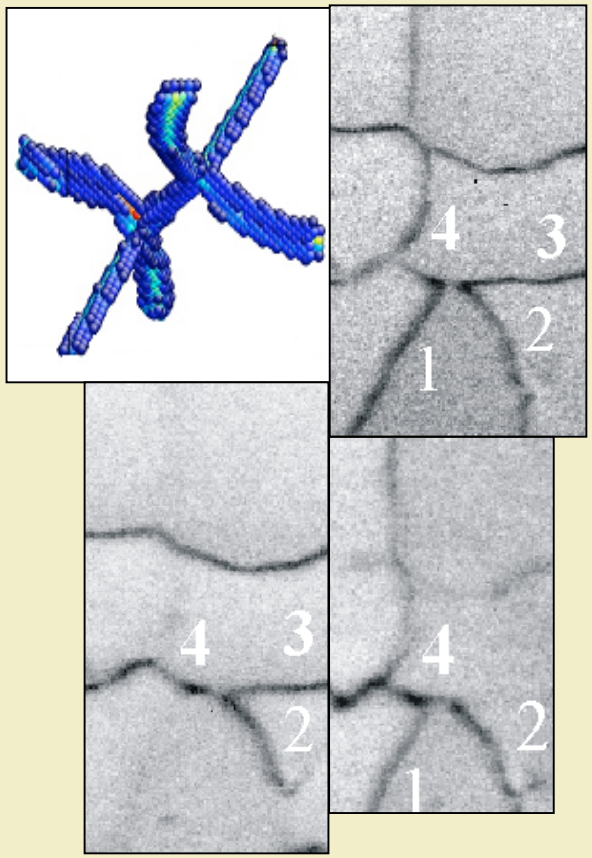




M-junctions hold dislocation strongly tie together enhancing the rate of dislocation multiplication

Existence of multi-junctions is experimentally verified

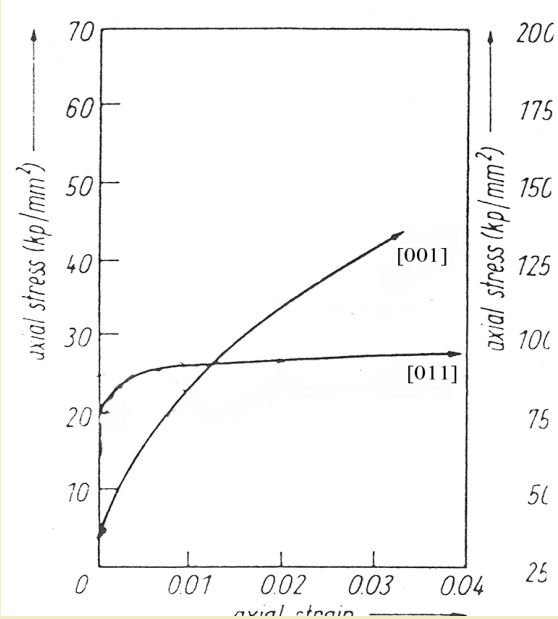
Multi-junctions have a unique TEM signature that allows them to be distinguished from other dislocation arrangements



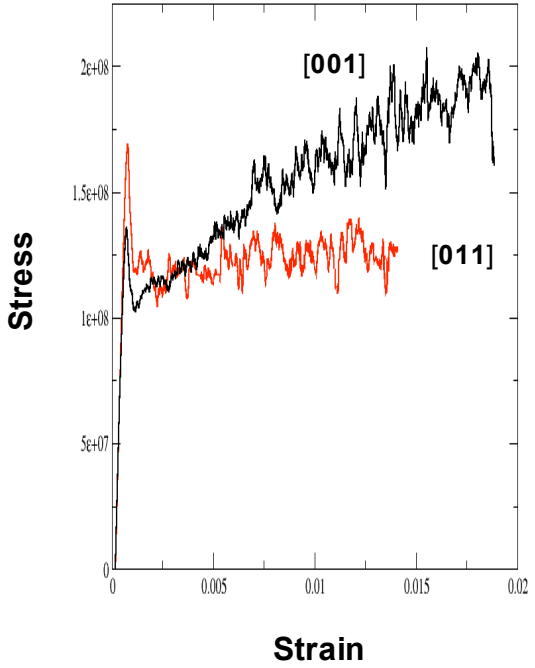
Multi-junctions are not rare and may occur frequently during certain plastic processes

Multi-junctions matter: orientation dependence of strain hardening in BCC metals

Experimental Observations

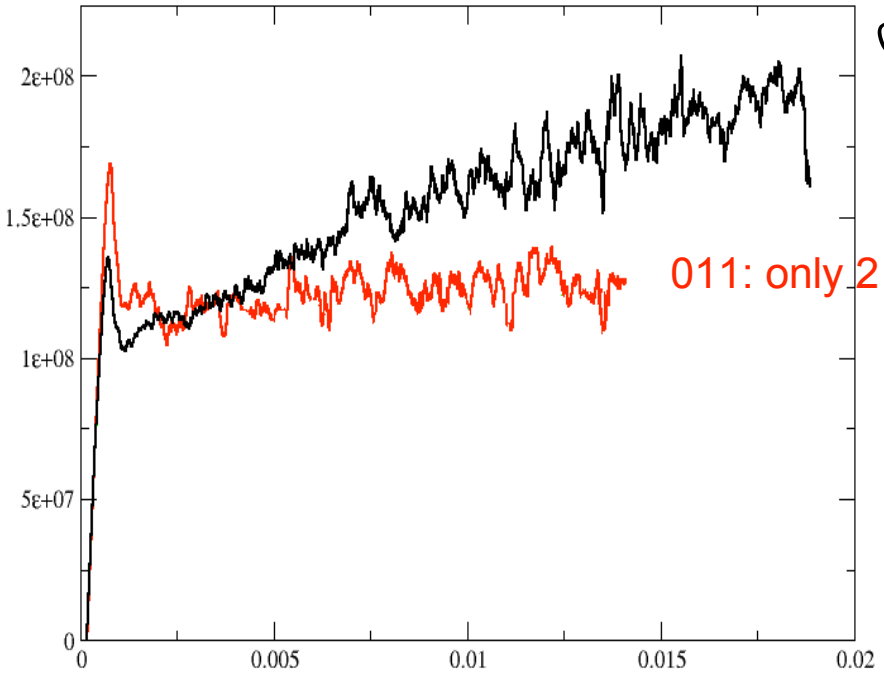


Simulation Results



With ParaDiS we are able to investigate the microstructural origins of this behavior

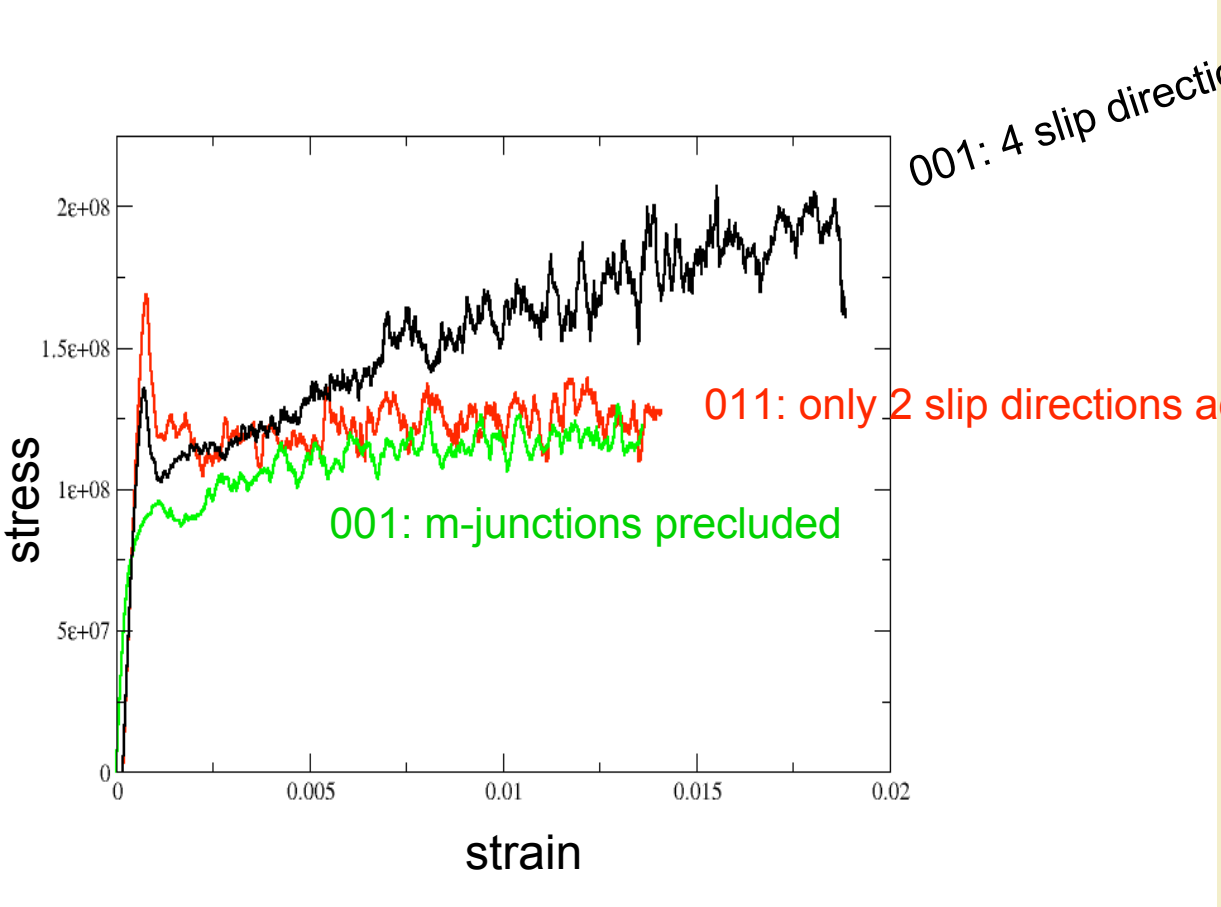
Do m-junctions matter for strain hardening?



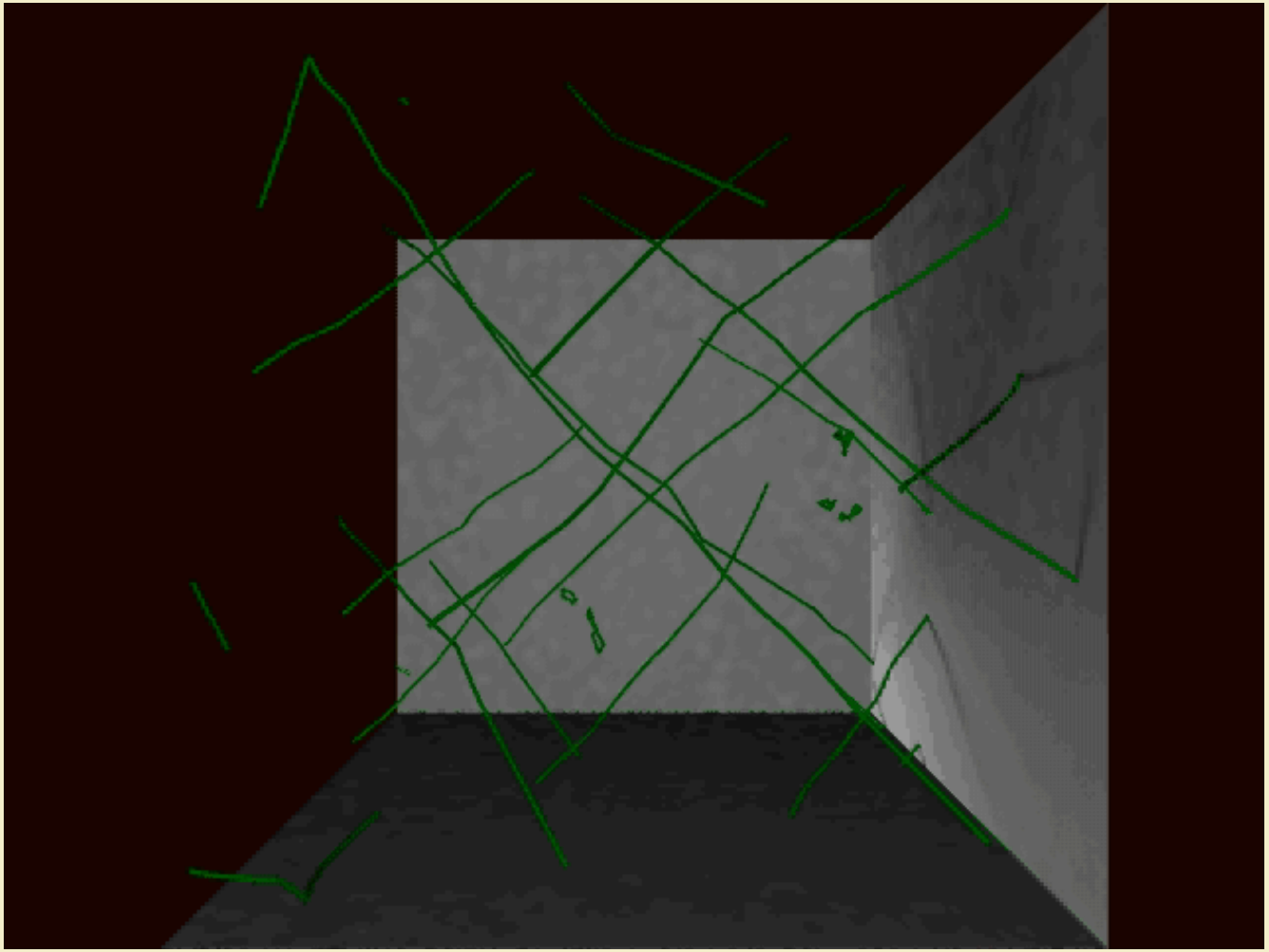
001: 4 slip directions

011: only 2 slip directions active

Yes, they do


001: 4 slip directions
011: only 2 slip directions active
001: m-junctions precluded
stress
strain
2ε+08
1.5ε+08
1ε+08
5ε+07
0
0
0.005
0.01
0.015
0.02

Growth of m-junction network



Movie by Rich Cook

ParaDiS connects dislocation physics to material strength

Overcomes computational limits through massively parallel computing

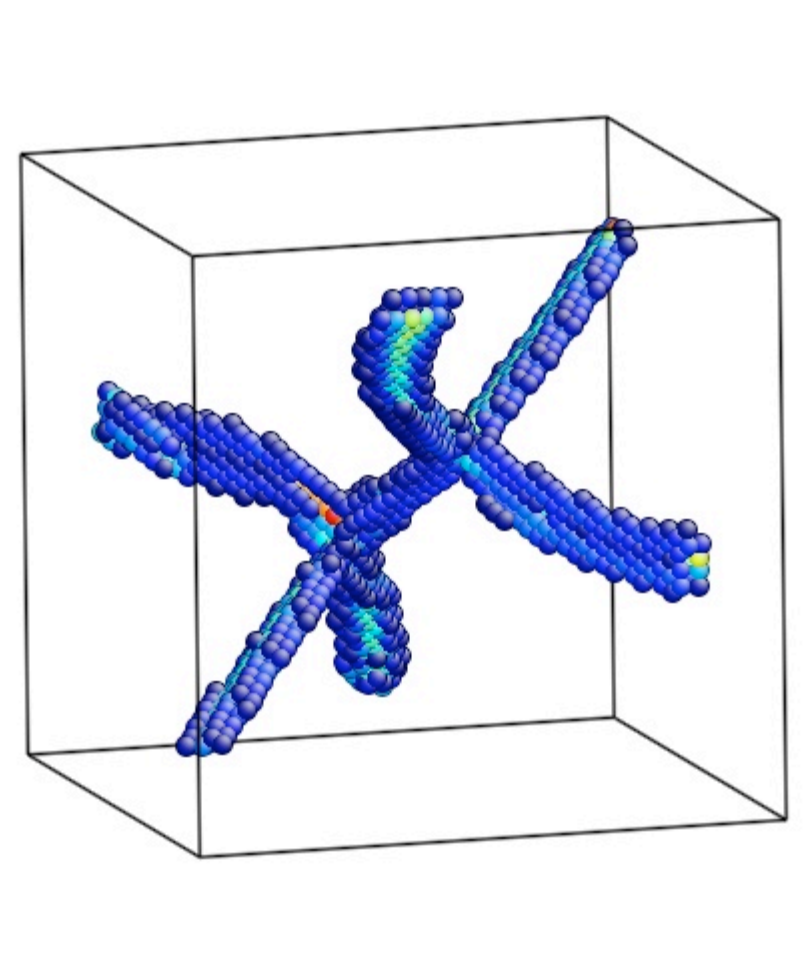
Enables discovery science

A computational laboratory for investigations of the origins of material strength

A virtual *in situ* microscope for observations of microstructural causes of strength

Extra slides

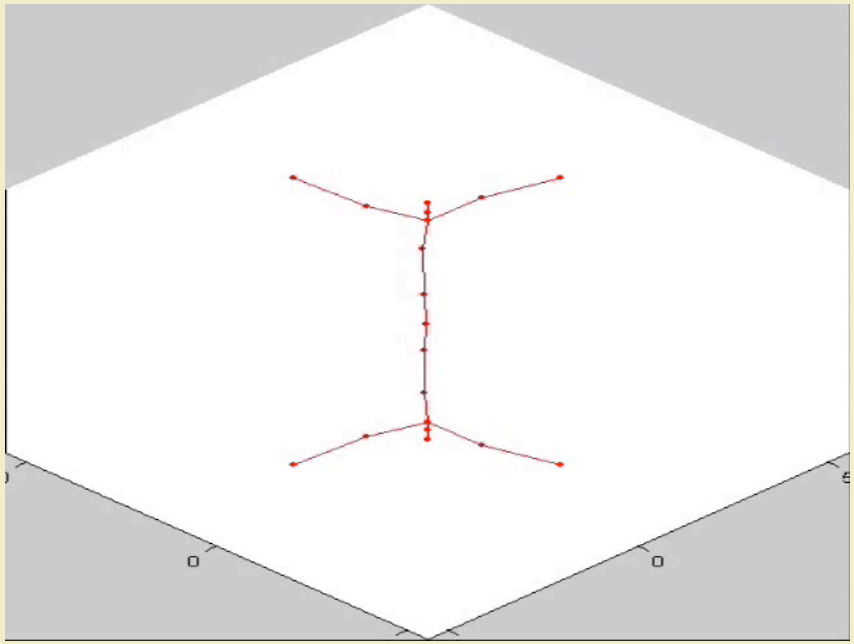
Atomistic simulations confirm the mechanism



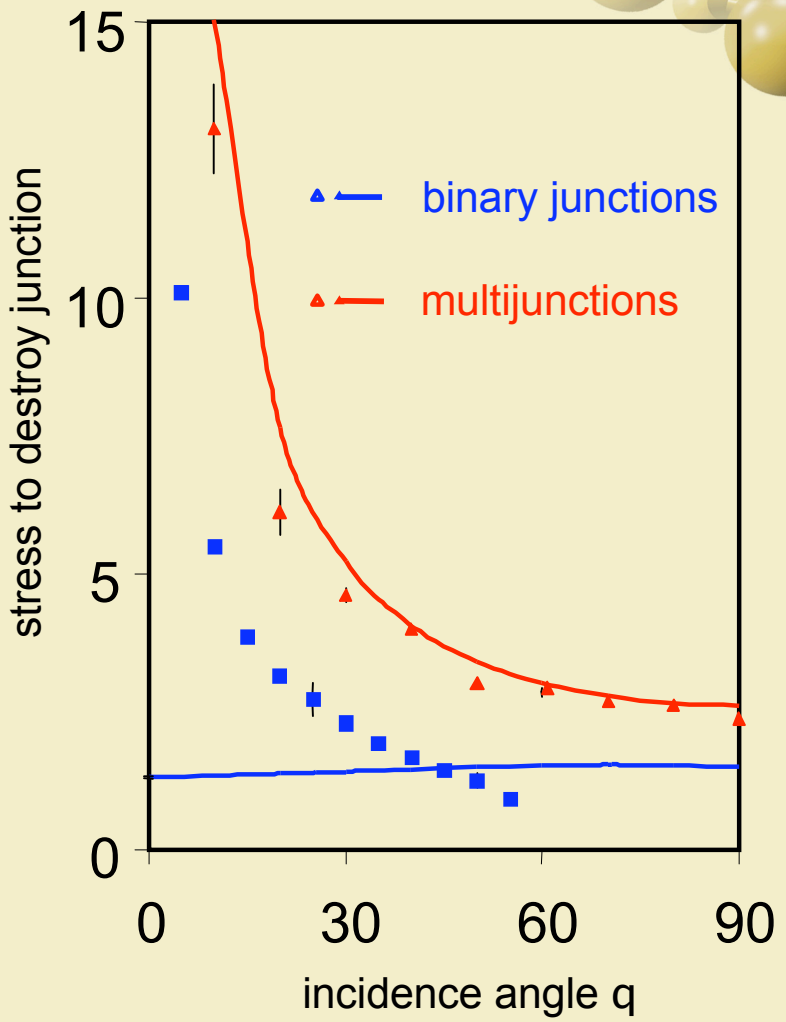
Conjugate gradient relaxation produces a multi-junction

Multi-junctions are strong obstacles to dislocation motion that are not easily overcome

Multi-junctions are 4x stronger than common binary junctions



Multi-junctions act as regenerative sources of dislocation multiplication



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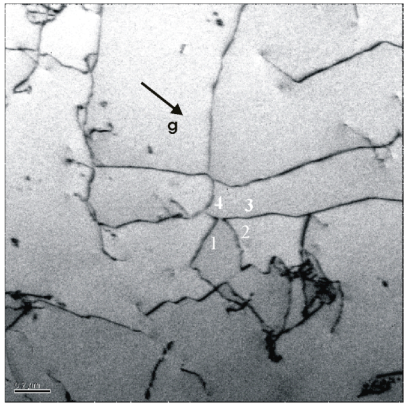
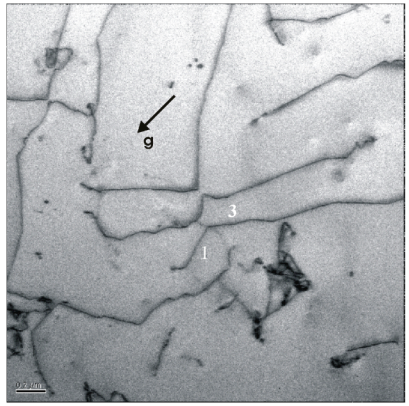
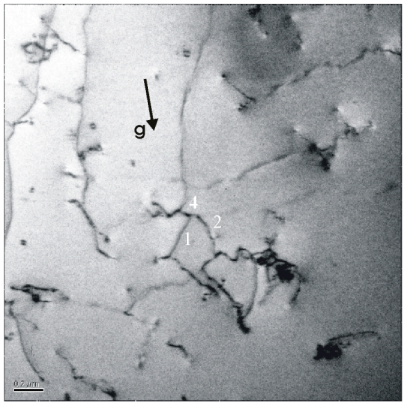
Multi-junctions have a unique TEM signature that allows them to be distinguished from other dislocation arrangements



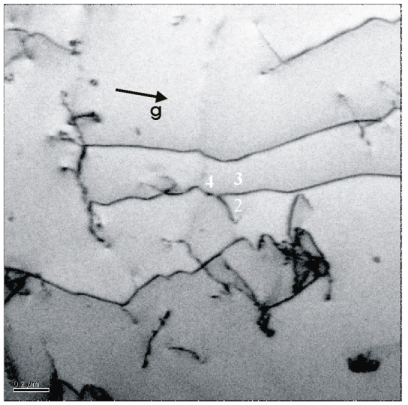
Z ≈ [-101], **g** = [020]



Z ≈ [-101], **g** = [101]



Z ≈ [-101], **g** = [121]



Z ≈ [-101], **g** = [-12-1]

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